Benchmarking atomic processes and atomic spectra for the modeling of EUV sources

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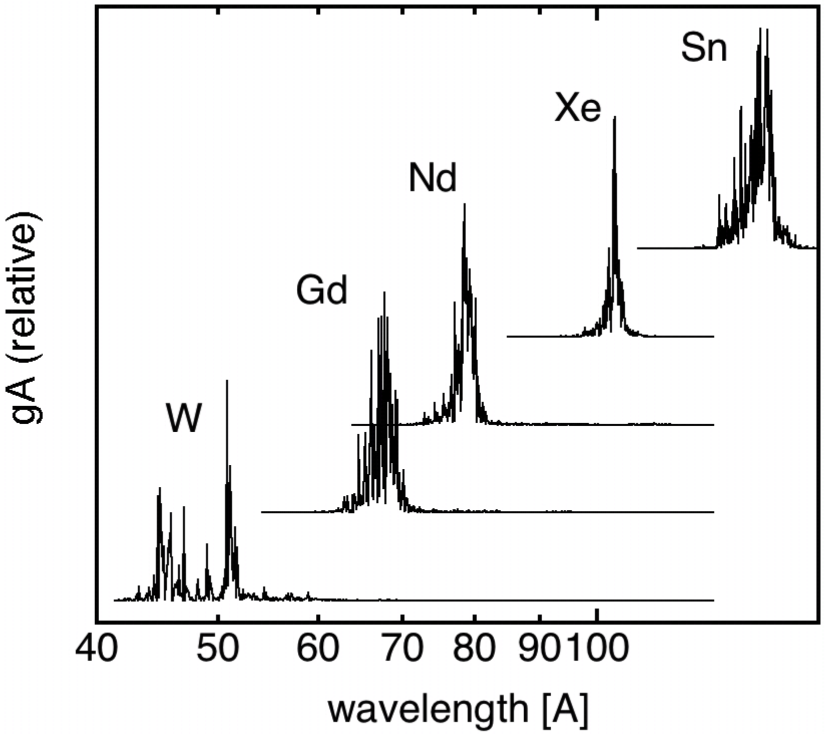
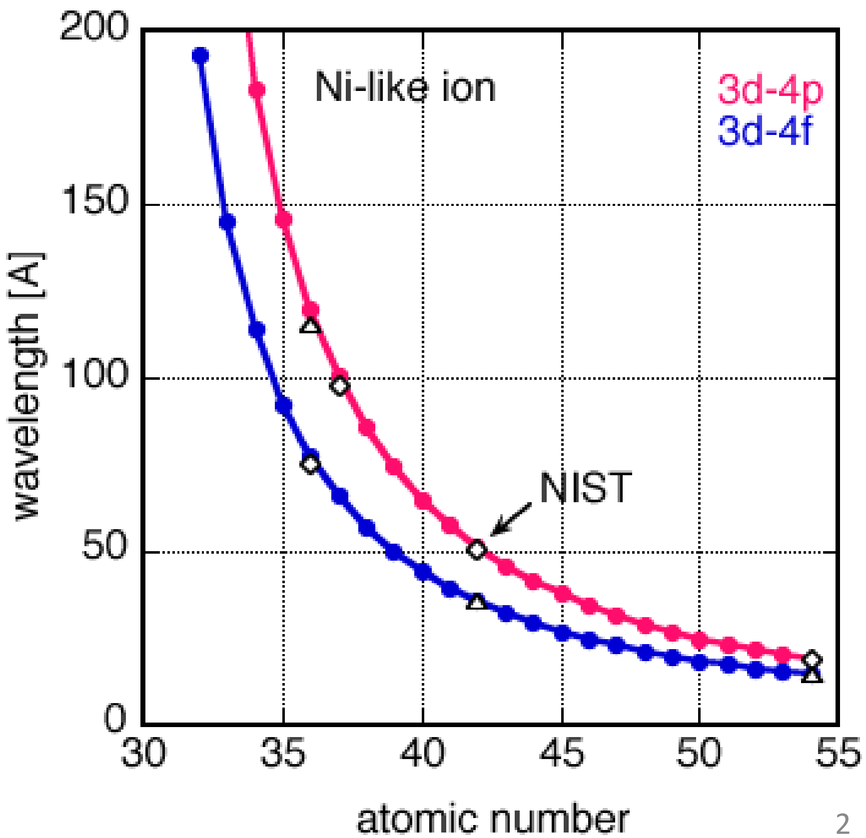
Previous report

EUV source is scalable to λ=6.5nm using Gd/Tb plasmas, but higher Te(≈100eV) is required.

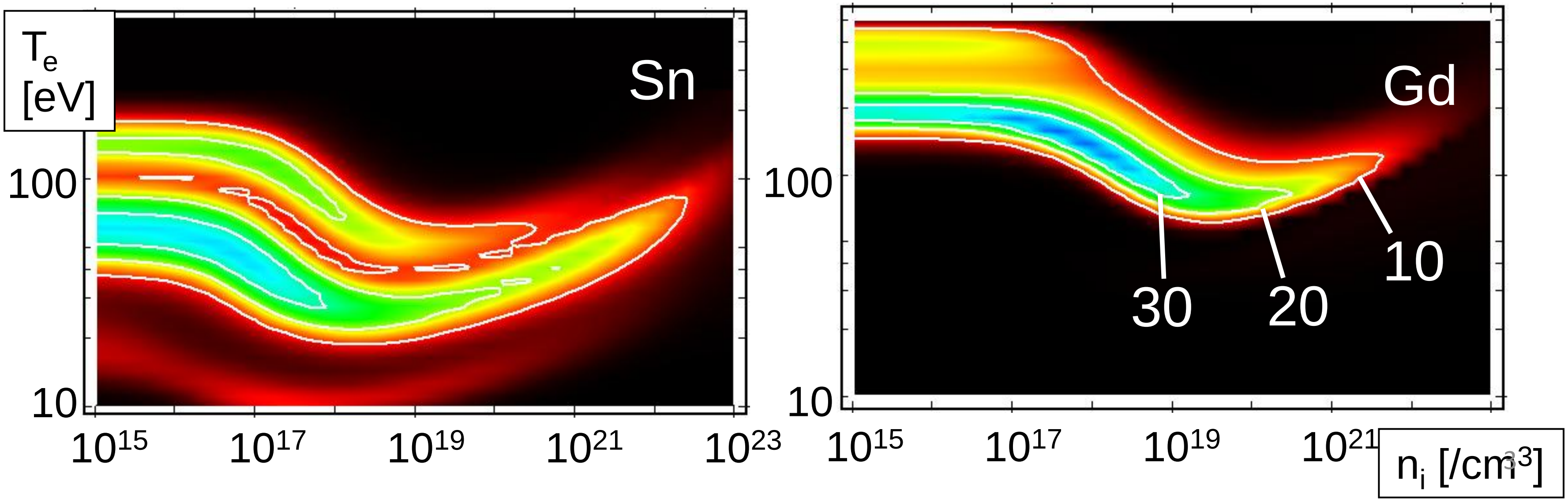


Shorter wavelength source may be realized also using Ni-like Kr.



Motivation

- Optimization based on radiation-hydrodynamics model relies on the accurate atomic data and atomic model.
- To predict emission from new fuel, the model should have higher accuracy.



Motivation

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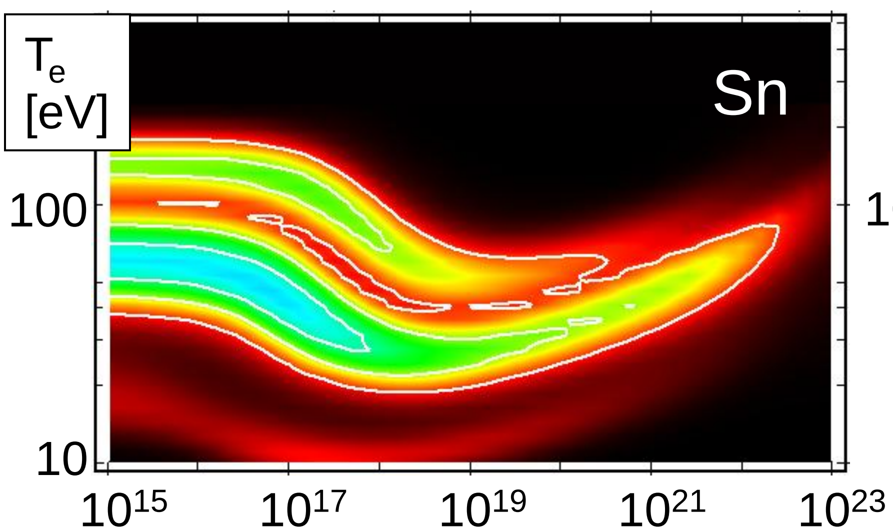
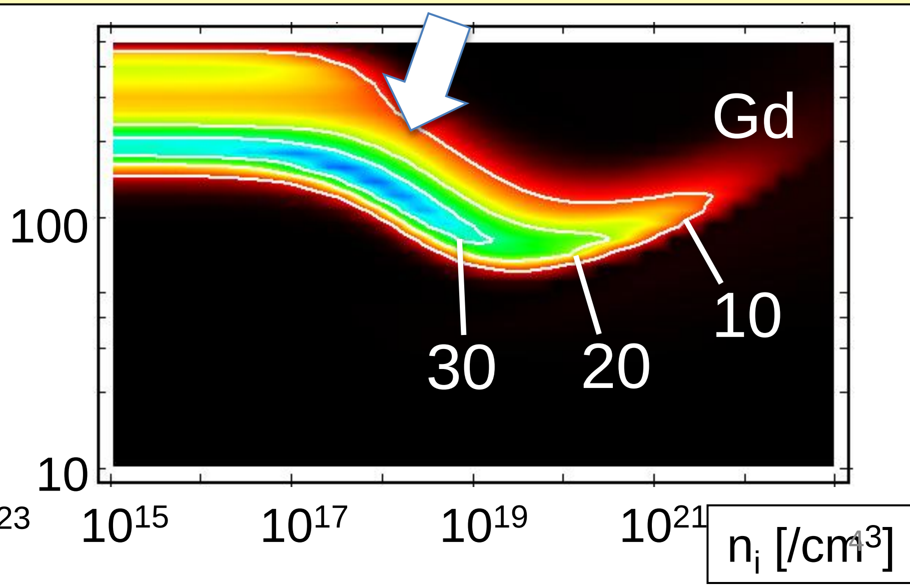
6.7nm source is operated at high T_e; effect of non-equilibrium (nLTE) atomic process is more pronounced.





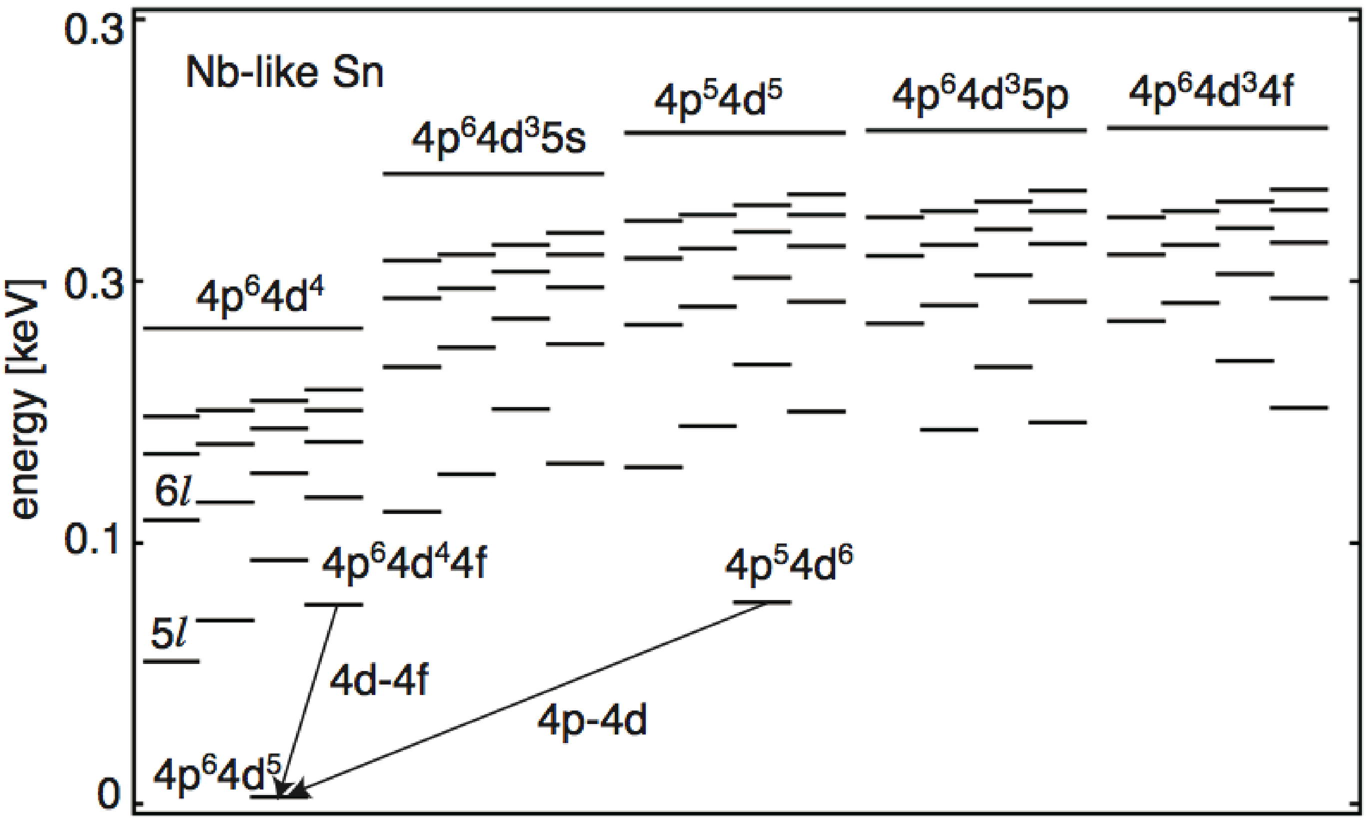
Topics

- Problems concerning to the atomic model identified through studies of EUV source.
- nLTE kinetics workshop activities for the validation of the atomic model.
- New method based on genetic algorithm (GA) for the improvement of atomic model (preliminary).

Requirements for the atomic model (1)

CR model should include a large number of energy levels

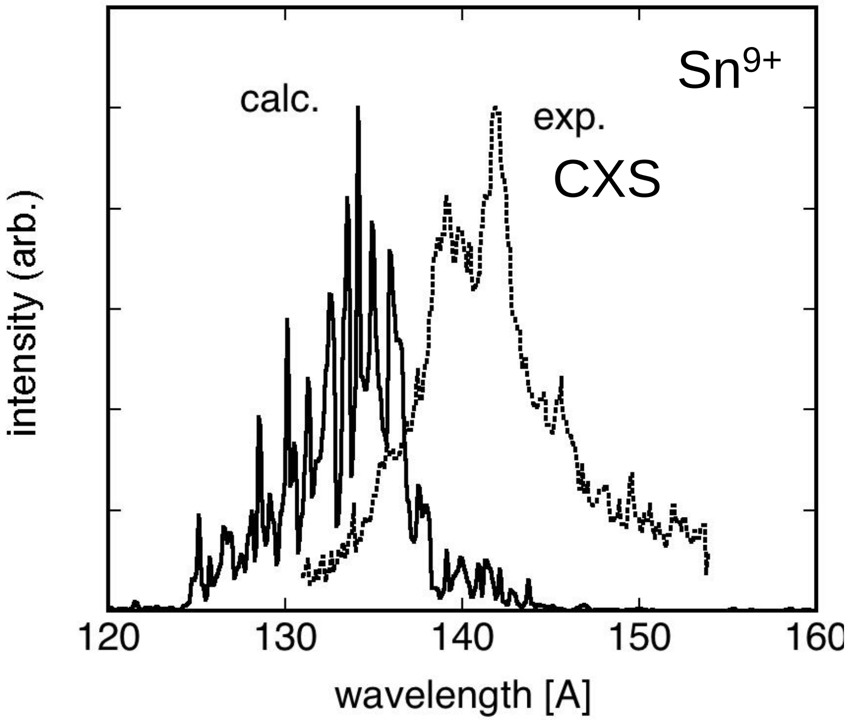
- For calculation of ion abundance and population.
- Take satellite lines from excited states into account.

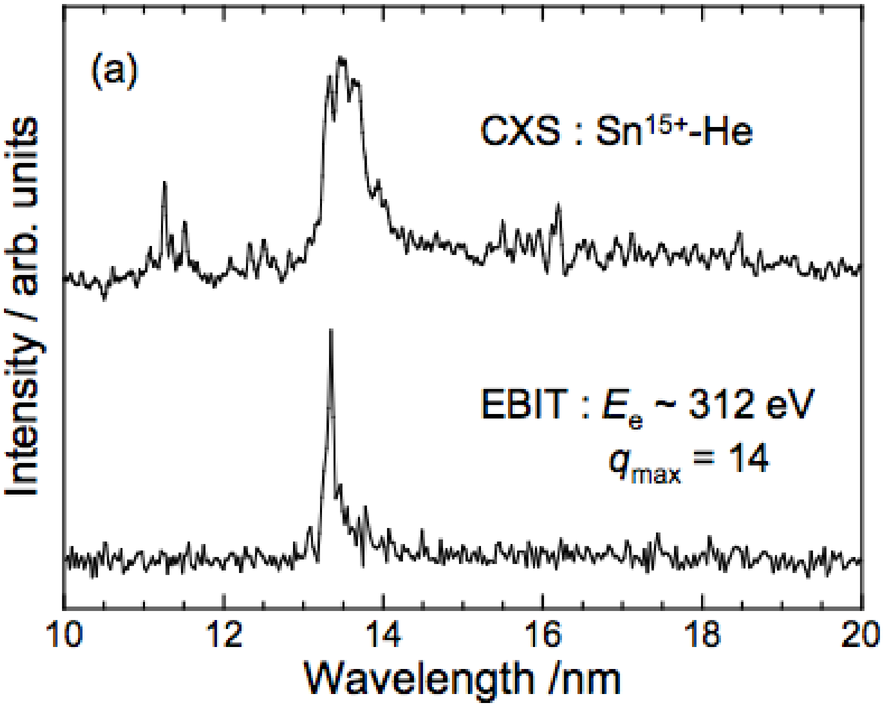


Requirements for the atomic model (2)

Accurate wavelength and transition probability data is required to calculate spectrum and efficiency.

- Calculated wavelength is corrected after comparison with experimental spectrum.





H. Ohashi, et al. J. Phys. Conf. Ser. 163, 012071(2009).

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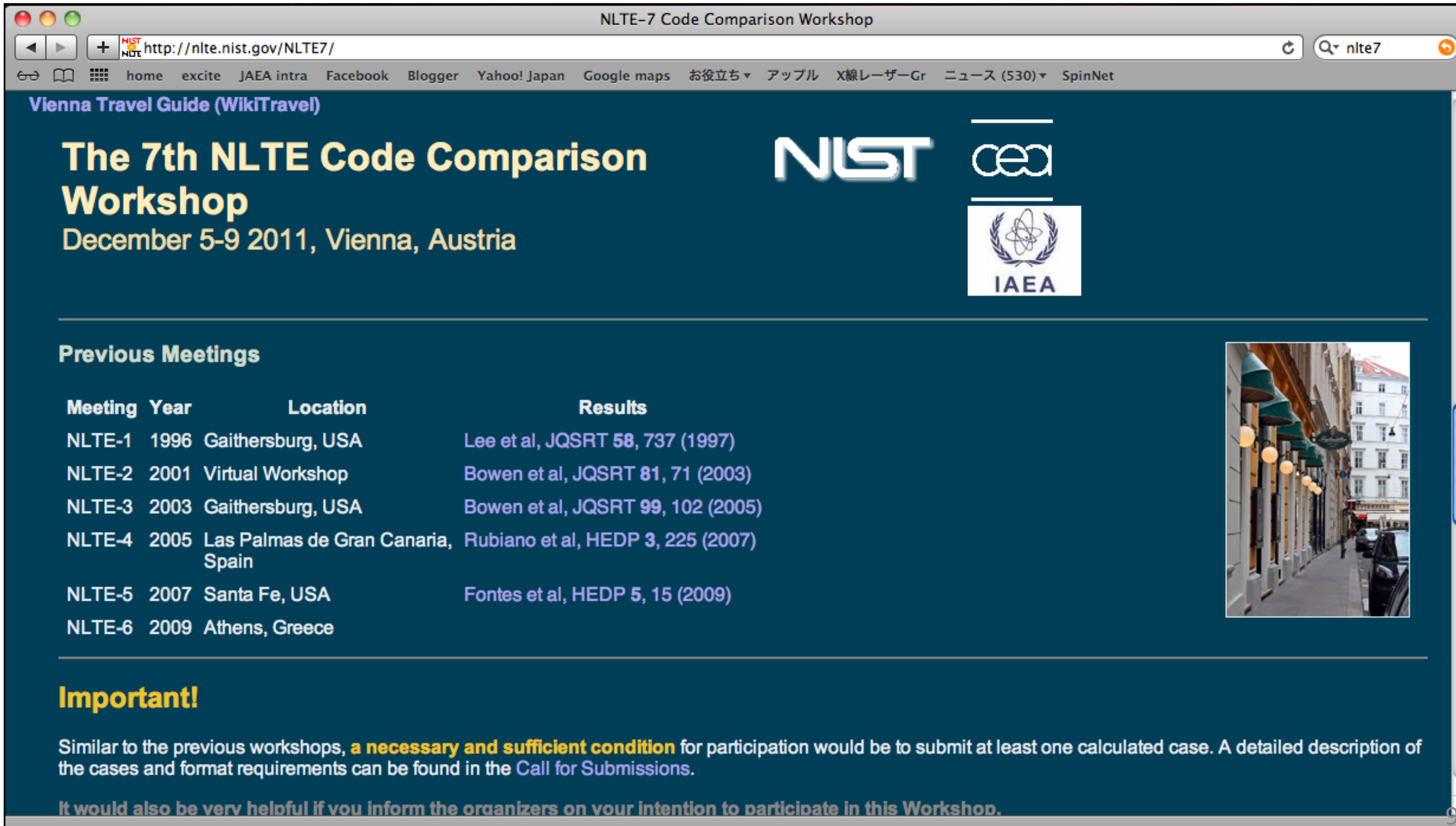
NLTE workshop

6 workshops dedicated to improvement of CR model have been held since 1996.



NLTE-7 Code Comparison Workshop

http://nlte.nist.gov/NLTE7/

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Vienna Travel Guide (WikiTravel)

The 7th NLTE Code Comparison Workshop

December 5-9 2011, Vienna, Austria

Previous Meetings

Meeting	Year	Location	Results
NLTE-1	1996	Gaithersburg, USA	Lee et al, JQSRT **58**, 737 (1997)
NLTE-2	2001	Virtual Workshop	Bowen et al, JQSRT **81**, 71 (2003)
NLTE-3	2003	Gaithersburg, USA	Bowen et al, JQSRT **99**, 102 (2005)
NLTE-4	2005	Las Palmas de Gran Canaria, Spain	Rubiano et al, HEDP **3**, 225 (2007)
NLTE-5	2007	Santa Fe, USA	Fontes et al, HEDP **5**, 15 (2009)
NLTE-6	2009	Athens, Greece	

Important!

Similar to the previous workshops, **a necessary and sufficient condition** for participation would be to submit at least one calculated case. A detailed description of the cases and format requirements can be found in the Call for Submissions.

It would also be very helpful if you inform the organizers on your intention to participate in this Workshop.

- Cases are chosen for each workshop.
- Participants submit calculations and the results are compared with each other during the workshop.

Element	Case ID	Total # of Points	Parameter	Grid	# of Points
Detailed NLTE case (proposed at NLTE-3); comparison with the benchmark theoretical results					
Carbon	C	16	T_e	3, 5, 7, 10	4
			N_e	10^{13}, 10^{15}, 10^{17}, 10^{19}	4
The same case (almost) as in NLTE-3; non-Maxwellian; **test the progress since NLTE-3**					
Argon	Ar	24	T_e	50, 100, 300, 600	4
			N_e	10^{12}, 10^{18}, 10^{23}	3
			T_2	10 000	
			% of T_2 in N_e	0 and 10%	2
Astrophysical photoionization case; Planckian radiation field					
Iron	Fe	25	T_e	15, 30, 60, 150, 300	5
			N_e	10^7	1
			T_{rad}	15, 50	2
			U_x	0, 0.1, 10	3
			Spectrum	10-1000 eV, ΔE = 1 eV (for T_e = 30 and 150 eV only)	991
EUV lithography; includes optically thick case; spectrum emission; exp. data available					
Tin	Sn	50	T_e	20, 25, 30, 35, 40	5
			N_e	10^{18}, 5×10^{18}, 10^{19}, 5×10^{19}, 10^{21}	5
			Spectrum	**100–180** Å, $\Delta\lambda$ = **0.02** Å	4001
			Opacity	**r = 0** and **0.1** mm; **L** = 5r	2
				Spectrum for N_e = 5×10^{18} only	
Radiation power loss case					
Xenon	Xe	27	T_e	10, 20, 50, 100, 200, 500, 1000, 2000, 5000	9
			N_e	10^{14}, 10^{18}, 10^{22}	3
Comparison with experimental data; Planckian radiation field					
Gold	Au	48	T_e	400, 870, 1400, 2000, 2500, 5000	6
			N_e	3×10^{20}, 10^{21}, 3×10^{21}, 10^{22}	4
			T_{rad}	0, 175	2
			Spectrum	**2.8–4.4** Å, $\Delta\lambda$ = **0.001** Å	1601

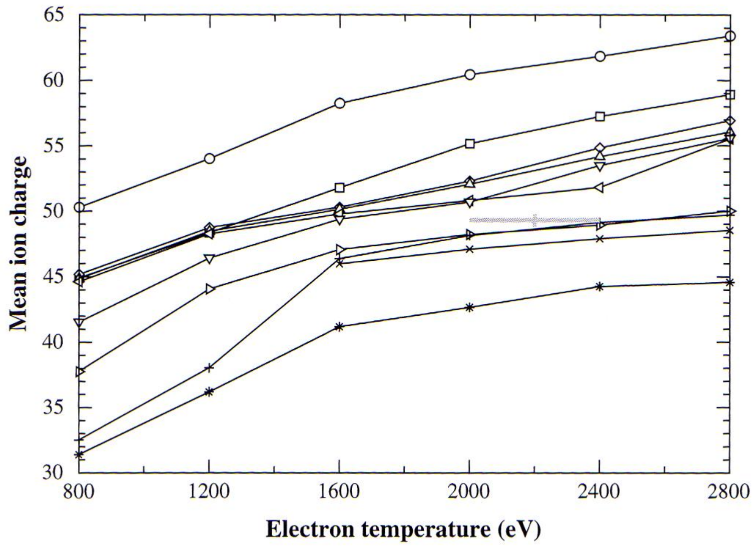
C, Al, Ar: laser fusion

Fe: astrophysics

Sn: EUV (NLTE-5)

W: magnetic fusion

NLTE-1, Au: $n_e = 10^{20}/cm^3$



Agreement of zbar has improved significantly for complex ions, which supports the accuracy of the calculation of Sn.

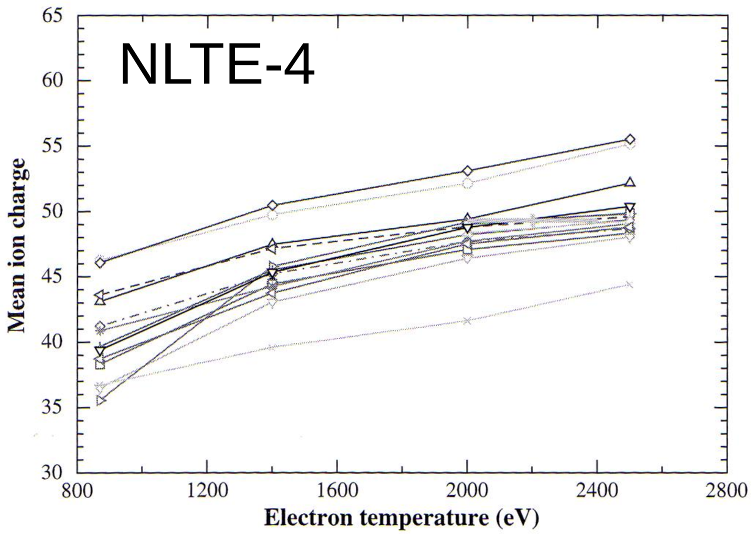
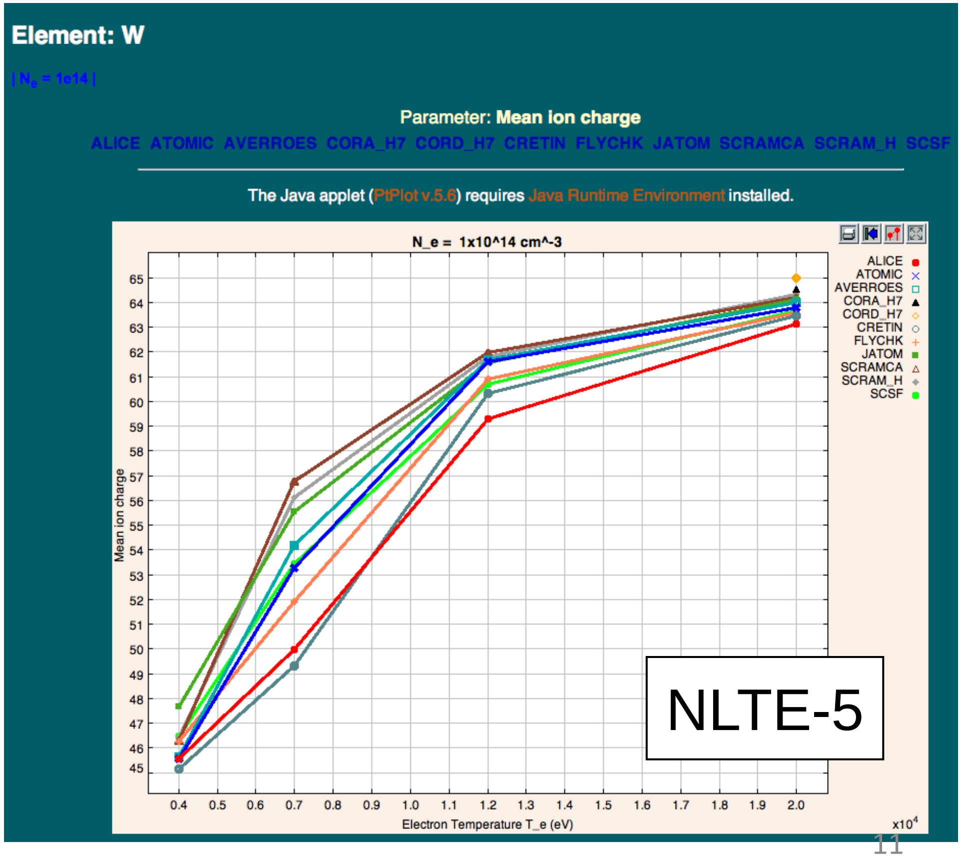


Fig. 9. Mean ion charge for Au as a function of T_e. Up: NLTE-1 results, $N_e = 10^{20}$ cm^{-3}; down: NLTE-4 results, $N_e = 3 \times 10^{20}$ cm^{-3}. The experimental value at $T_e = 2200$ eV, $N_e = 6 \times 10^{20}$ cm^{-3}, is $\overline{Z} = 49.3 \pm 0.5$ [30], in approximate agreement with the theory.



Difficulty of benchmarking calculation of spectrum

- Observed spectrum depends on T_e and n_e, and their spatial and temporal evolution.
- Spectrum depends on opacity.
- Calculation includes significant uncertainties in wavelength and transition probability of emission lines, rate coefficients of collisional and radaitive processes.

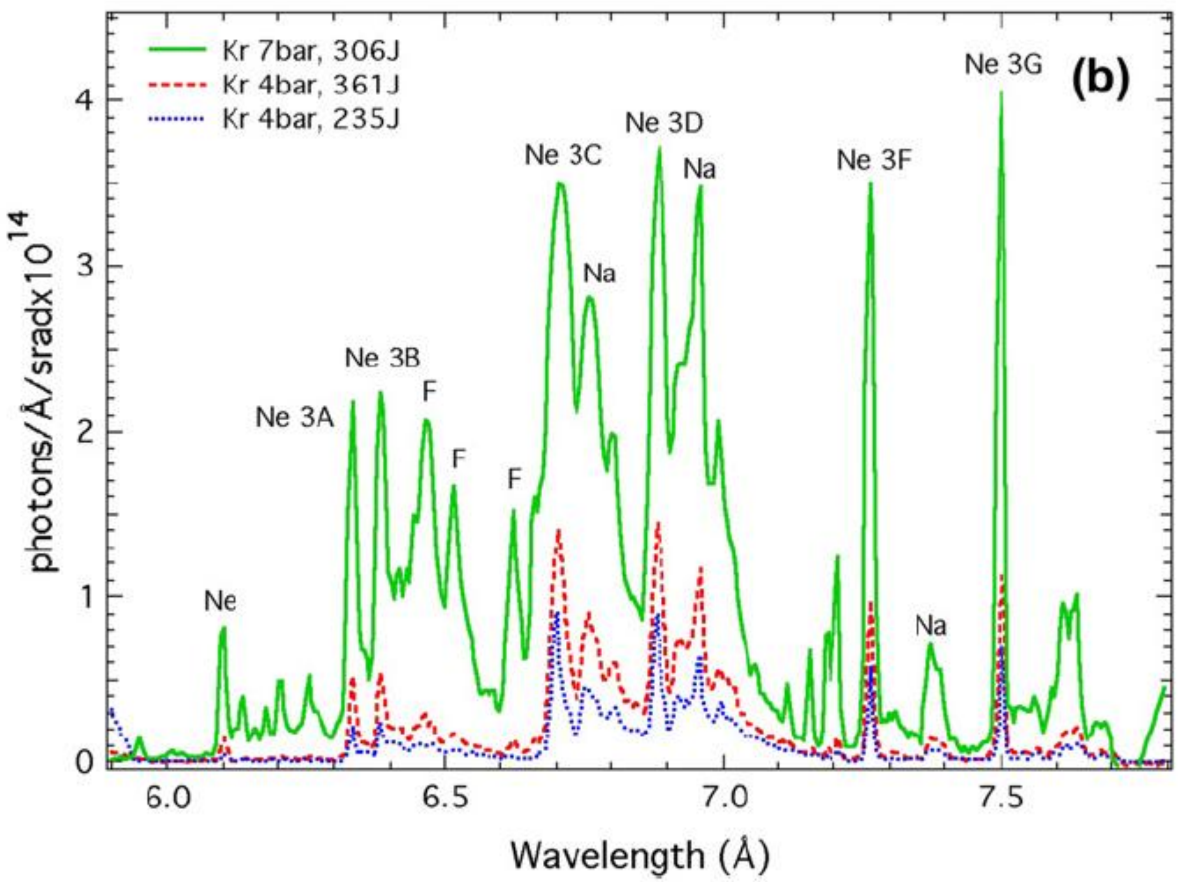
  - Identification of emission line is difficult.
  - Calculation may be incorrect even it agrees with experiment at a specific condition.

$\downarrow$

Optimization problem with a large number of dimensions

Benchmarking spectrum in NLTE-7 (Dec. 2011)

Comparison of emission from near Ne-like Kr in a wavelength region 6.0-7.6nm will be carried out.



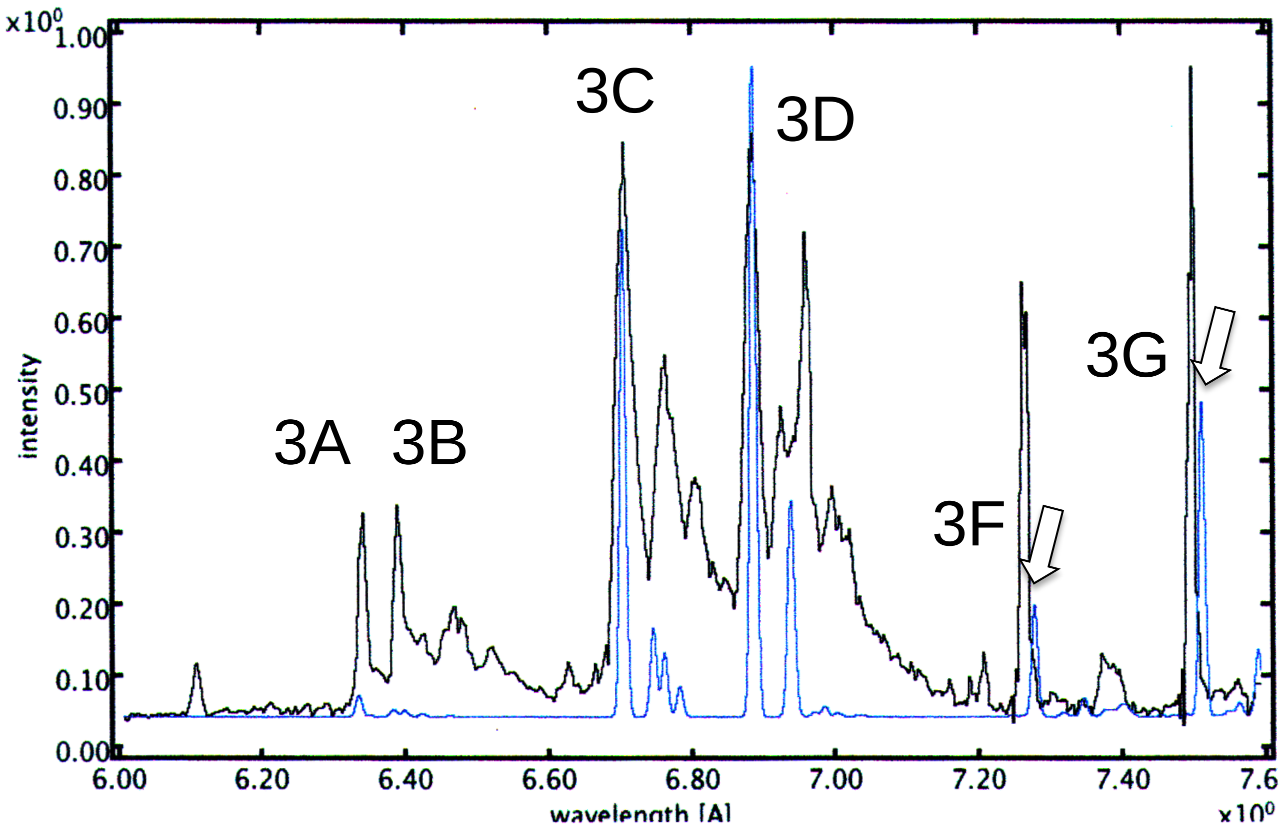
2s-3p
3A (2s 1/2, 3p 3/2) J=1
3B (2s 1/2, 3p 1/2) J=1

2p-3d
3C (2p 1/2, 3d 3/2) J=1
3D (2p 3/2, 3d 5/2) J=1

2p-3s
3F (2p 1/2, 3s 1/2) J=1
3G (2p 3/2, 3s 1/2) J=1

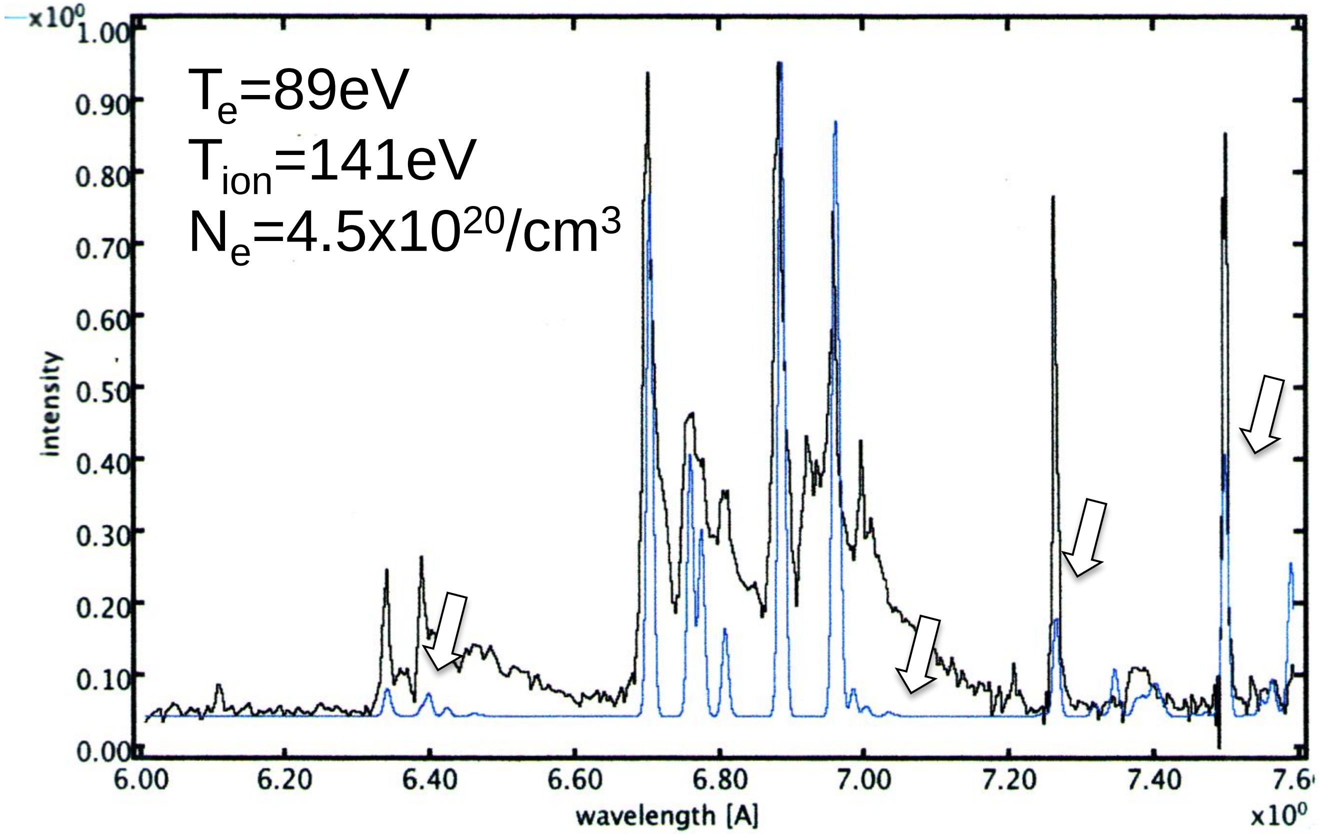
Difference of calculated and measured spectrum

- Spectrum is calculated including Na-like (2p^6nl, 2p^{5}3snl, 2s3snl), Ne-like (2snl, 2pnl), Ne-like (2s2p^5nl, 2p^4nl) ions.
- Wavelength of 3F/G differs from experiment for 13mÅ.

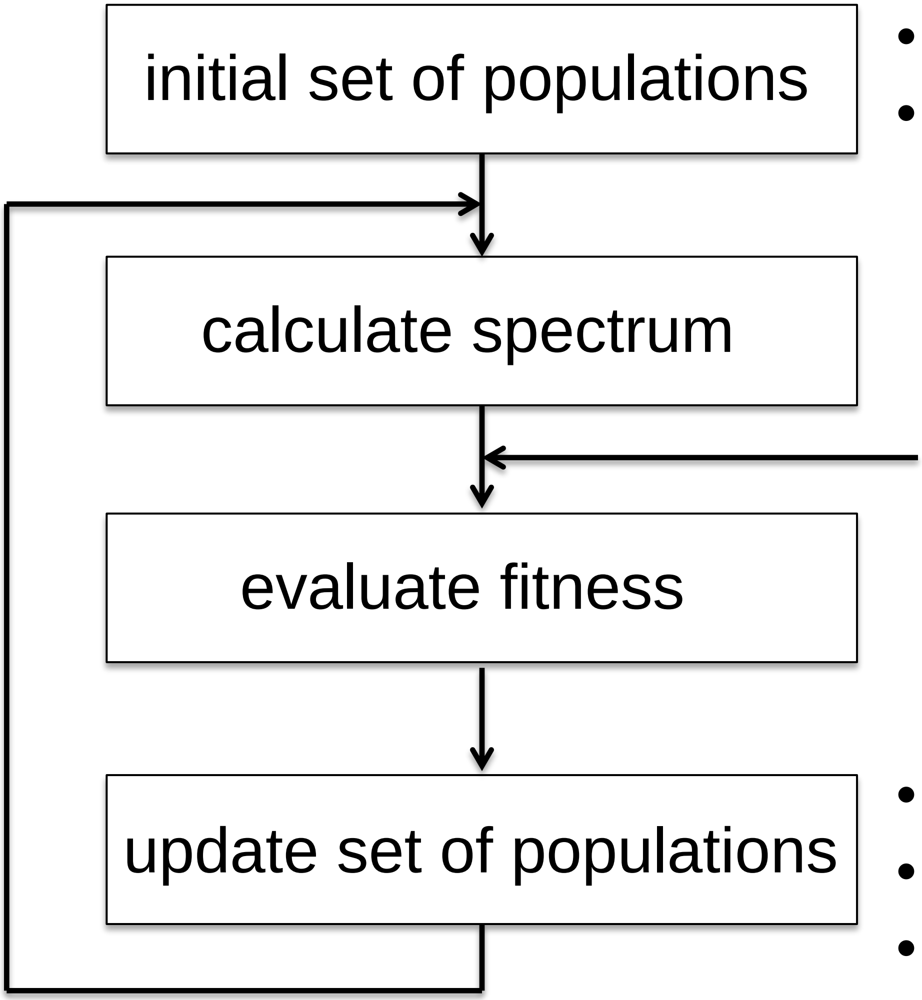


Calculation assuming quasi thermo-equilibrium

- T_{ion}, T_e and n_e are optimized to obtain best agreement.
- Wavelength of major lines are corrected.
- Calculation cannot reproduce measured line ratio.



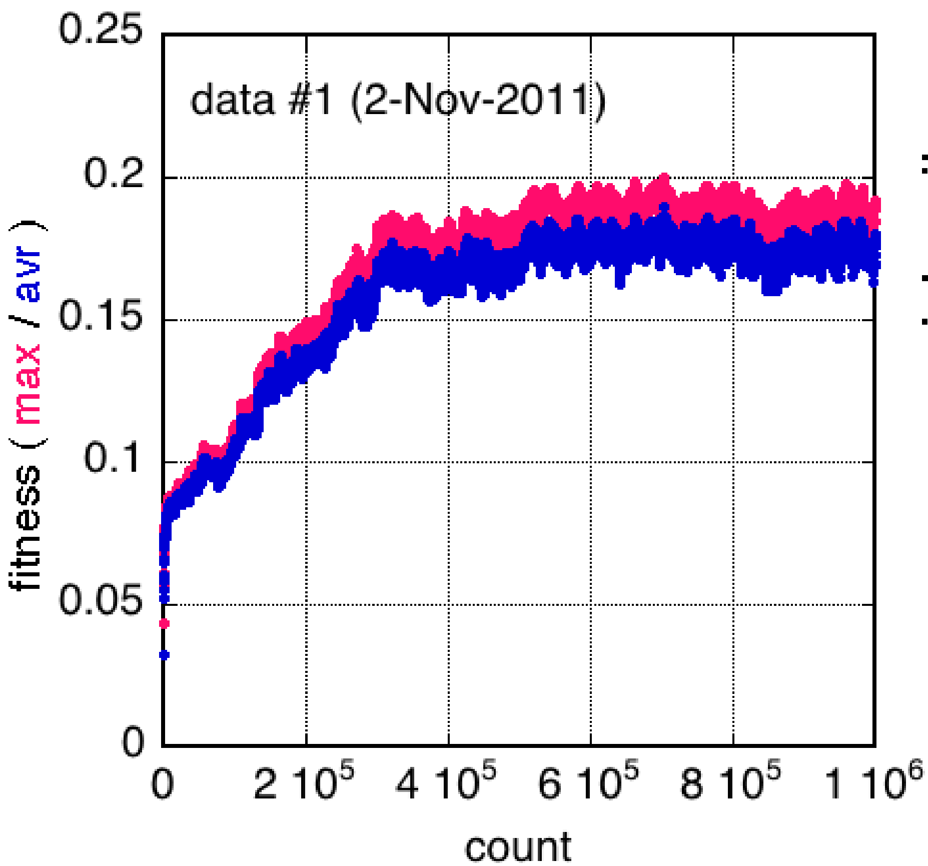
Population which gives best agreement with experimental spectrum is estimated using genetic algorithm

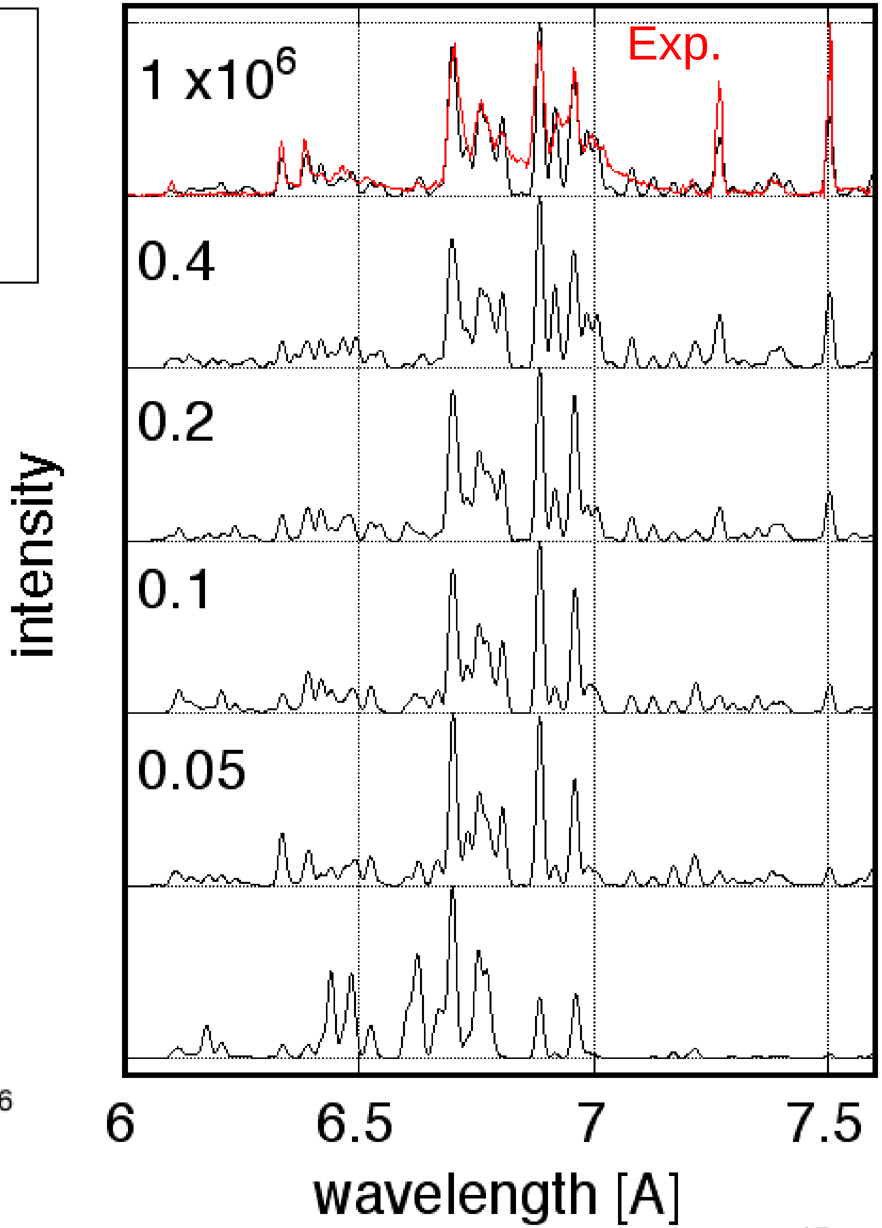


- 115 levels
- 500 sets of populations

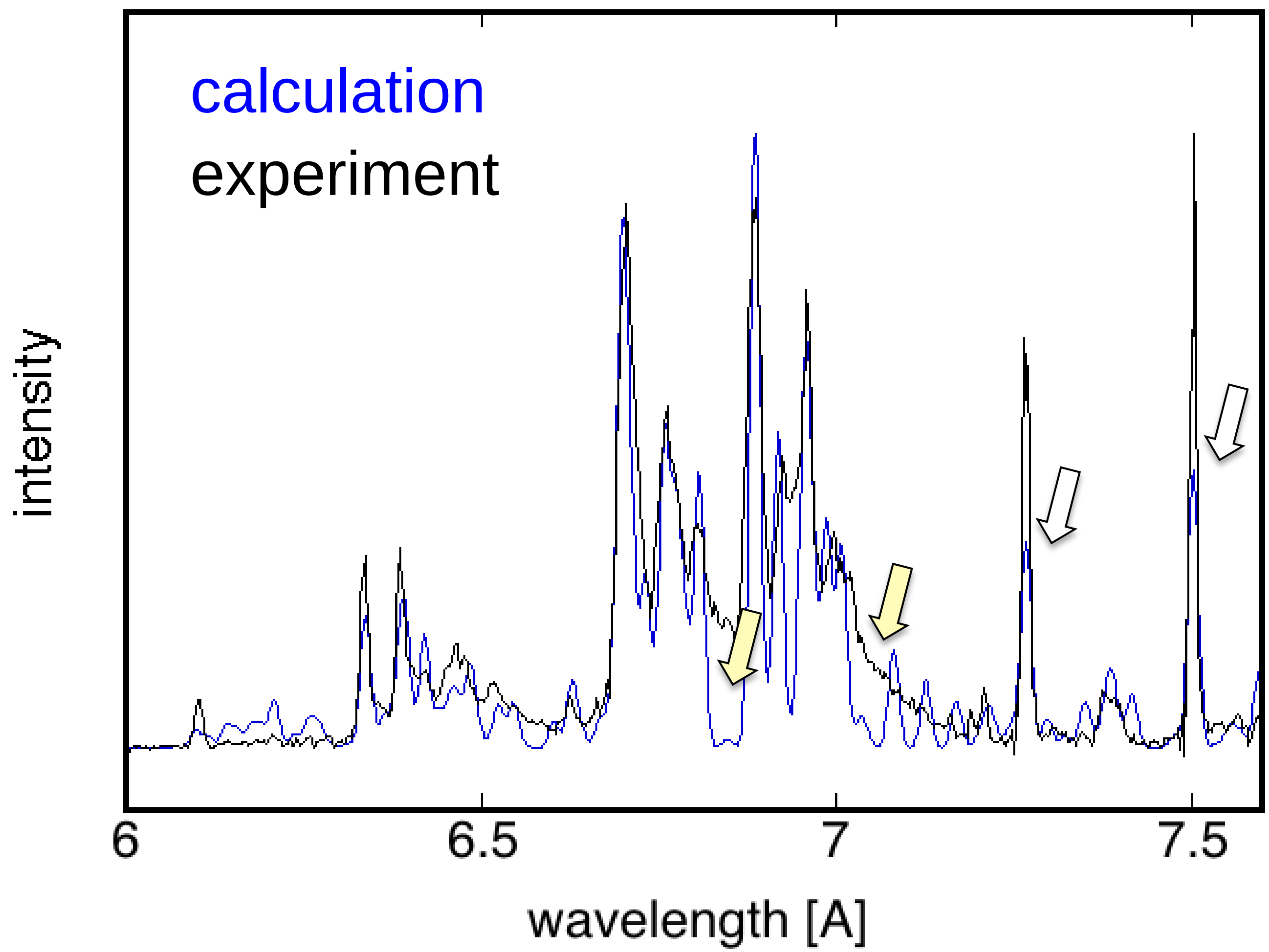
- selection
- crossover
- mutation

Estimated spectrum approaches experiment after a large number of iterations.





- Better agreement with experiment is obtained.
- Calculation does not reproduce tail of the spectrum which may arise from satellite lines from excited states.



Summary

- Present status of benchmarking the model of EUV source in terms of atomic process is presented.
- CR-model has become more accurate through NLTE workshop, but calculation of spectrum still needs improvement.
- GA is shown to be useful for estimating population which gives the experimental emission spectrum.
- Simultaneous optimization of population and wavelength, GA may be useful to identify emission lines and correct the calculated wavelength.

- Wavelength of the line can be determined by simultaneous optimization of population and wavelength.